



Approximations of Kinetic Equations

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17-19 Aug 2009

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2 Closures









Modelling Beyond Equilibrium ...

Particle collisions drive system into equilibrium

 \longrightarrow equilibrium thermodynamics.

Small scales — few collisions

Scaling Parameter:

Knudsen Number $\varepsilon = \frac{\text{mean free path} \equiv \lambda}{\text{system size} \equiv L}$





porous media



micro heat exchanger



micro fuel cell

Kinetic Theory

provides a general modeling framework for multi-scale micro-macro transitions:



- * $f_{\mathbf{x},t}(\mathbf{c})dc =$ gives number density of particles in $[\mathbf{c}, \mathbf{c} + d\mathbf{c}]$.



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provides a general modeling framework for multi-scale micro-macro transitions:



Macroscopic: (moment equations)

$$\rho(\mathbf{x},t) = m \int_{\mathbb{R}^3} f d\mathbf{c}, \qquad F_{i_1...i_n}(t,\mathbf{x}) = m \int_{\mathbb{R}^3} c_{i_1}...c_{i_n} f_{\mathbf{x},t}(\mathbf{c}) d\mathbf{c}$$

Complexity reduction $f_{\mathbf{x},t}(\mathbf{c}), \mathbf{c} \in \mathbb{R}^3 \longleftrightarrow \{F_{i_1...i_n}(\mathbf{x},t)\}_{n=0,1,...,N}$. Corresponds to special spectral method with monomials $c_{i_1}...c_{i_n}$ as test functions.

$$\begin{array}{rcl} \partial_t F + \partial_i F_i &=& 0\\ \partial_t F_i + \partial_j F_{ij} &=& 0\\ \partial_t F_{kk} + \partial_i F_{ikk} &=& 0 \end{array} \right\} \quad \text{cons. laws} \\ \partial_t F_{} + \partial_k F_{k} &=& P_{ij}\\ \partial_t F_{ijk} + \partial_l F_{ijkl} &=& P_{ijk}\\ \vdots & \ddots \end{array}$$

Fluid Variables: $F = \rho, F_i = \rho v_i, F_{kk} = 3\rho\theta + \rho v_k^2,$ $F_{\langle ij \rangle} \sim \sigma_{ij}, F_{ikk} \sim q_i$

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provides a general modeling framework for multi-scale micro-macro transitions:



Transition: Modelling

$$F_{i_1...i_Nk} \approx \int_{\mathbb{R}^3} c_{i_1}...c_{i_N} c_k \mathbf{f}^{(\text{model})} \left(\lambda_{\alpha} [\mathbf{F}, \mathbf{F}_i, ..., \mathbf{F}_{i_1...i_N}](\mathbf{x}, \mathbf{t}), \mathbf{c} \right) d\mathbf{c}, \quad \alpha = 1, ..., N,$$

$$\lambda_{\alpha} \text{ any functional acting on } F_{i_1, ..., i_N} (\cdot, \cdot).$$

Goal: Find $f^{(model)}$ such that resulting system

$$\partial_t U + \operatorname{div} \mathcal{F}(U) = \mathcal{P}(U)$$

has nice mathematical properties (stability),
 and is physically accurate.

Low dimensional approximation of high dimensional problem.

Linearized Boltzmann

 $\partial_t f + \mathbf{c} \cdot \nabla f + \frac{1}{\varepsilon} K f = 0, \quad f_{\mathbf{x},t}(\cdot) \in V, \quad \text{Equilibrium: } \{f : Kf = 0\} = \ker(K) := V_0 \subset V.$

Parametrization of Equilibrium				
moments	$M:\mathbb{R}^m\ni\rho$	surjective →	$f_0 \in \ker K \equiv V_0$	distribution
distribution	$E_0:V i f$	surjective →	$ ho \in \mathbb{R}^m$ moments	

Features:

$$\triangleright \ E_0 M = id_{\mathbb{R}^m \to \mathbb{R}^m}.$$

- ▶ $V_{NE} := V \setminus V_0$: non-equilibrium phase space.
- ▶ $Q := ME_0 = id_{V_0} + 0_{V_NE} : V \rightarrow V_0$ (surjective) "euglibrium projection".
- $P := id Q = id_{VNE} + 0_{V0} : V \rightarrow V_{NE} \text{ (surjective)}$ "non-equilibirum projection".



Classical Closures

 $\partial_t f + c \partial_x f = -\frac{1}{\varepsilon} K f$

♦ Chapman-Enskog (1916) expansion in Knudsen number ε:



Classical Closures

$$\begin{array}{c} \text{Closures}\\ \partial_t f + c \partial_x f = -\frac{1}{\varepsilon} K f \end{array}$$

♦ Chapman-Enskog (1916) expansion in Knudsen number ε:



♦ Grad: assume $f = M\rho + G\mu$. $\mu \in W \subset \mathbb{R}^s$, $G : \mathbb{R}^s \to V_{NE}$ arbitrary direction.

Grad's equations (1949)

$$\partial_t \rho + E_0 \mathbf{c} \cdot \nabla M \rho + E_0 \mathbf{c} \cdot \nabla G \mu = 0$$

$$\partial_t \mu + E_1 \mathbf{c} \cdot \nabla M \rho + E_1 \mathbf{c} \cdot \nabla G \mu + \frac{1}{\varepsilon} E_1 K G \mu = 0$$
 \bigoplus stable \bigcirc accuracy unclear

Scale Induced Closure [Torrilhon, Kauf, Levermore, Junk 2008; Struchtrup 2004]

Idea:

V1

Combine stability of Grad and accuracy of Chapman-Enskog: $f = M\rho + \varepsilon G\mu + \varepsilon^2 f_2$.

Separation of phase space into $V = V_0 \oplus V_{NE} = \underbrace{V_0}_{\text{equilibrium}} \oplus \underbrace{V_1^{\varepsilon}}_{1 \text{ st order NE}} \oplus \underbrace{V_2^{\varepsilon^2}}_{2 \text{ order NE}} \oplus \underbrace{V_1^{\varepsilon^2}}_{\text{higher NE}} \oplus \underbrace{V_1^{\varepsilon^2}}_{1 \text{ st order NE}} \oplus \underbrace{V_2^{\varepsilon^2}}_{1 \text{$



Equations

$$\partial_t \rho + E_0 \mathbf{c} \cdot \nabla M \rho - E_0 \mathbf{c} \cdot \nabla G \mu = 0$$
$$\partial_t \mu + E_1 \mathbf{c} \cdot \nabla M \rho - E_1 \mathbf{c} \cdot \nabla G \mu - \frac{1}{\varepsilon} E_1 K G \mu = 0$$

 \bigoplus accurate to 2^{nd} order.



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Vo

 $\mathbf{V_2}$

Scale Induced Closure

From kinetic equation: $G = -K^{\dagger} \mathbf{c} M D^{\dagger}$, $D^{\dagger} : \mu \mapsto \nabla \rho$

Equations

$$\partial_t \rho + E_0 \mathbf{c} \cdot \nabla M \rho - E_0 \mathbf{c} \cdot \nabla G \boldsymbol{\mu} = 0$$

$$\partial_t \mu + E_1 \mathbf{c} \cdot \nabla M \rho - E_1 \mathbf{c} \cdot \nabla G \mu - \frac{1}{\varepsilon} E_1 K G \mu = 0$$

 ♦ Theorem 1: [Torrilhon, Kauf, Levermore, Junk 2008/2009] Under moderate conditions, the equations (1) are of 2nd order if expanded in ε.
 → Generalization of Chapman-Enskog

Theorem 2: [Torrilhon, Kauf, Levermore, Junk 2008/2009] If K symmetric and positive semi definite, (1) features a convex entropy with associated negative definite entropy production.

→ stability

stable

 \bigoplus accurate to 2^{nd} order.

Generalizations to higher orders possible.

(1)

16 Discrete Velocity Model [Babovsky, Kauf 2008]

16 Velocities

Goal: Analyse abilities of different closures in simplified (1+1+2 dim) collision model.

Discrete velocity space:



Linearization and Fourier transform (in x):

$$\partial_t \hat{f}_j^k(t) - i \sum_{j=1}^{16} V_{ijk} \hat{f}_j^k(t) + \frac{1}{\varepsilon} \sum_{j=1}^{16} K_{ij} \hat{f}_j^k(t) = 0,$$

transport \equiv oscillation exact Solution: $\hat{\mathbf{f}}^{k}(t) = \exp[i \mathbf{k} \mathbf{V} - \frac{1}{\varepsilon} \mathbf{K}] \hat{\mathbf{f}}^{k}(0)$ interaction \equiv damping

Features of *K*:

 $\dim(\ker(K)) = 4 \qquad \qquad \triangleright \ \dim(V_1) = 3 \qquad \qquad \triangleright \ \dim(V_2) = 9$

Low dimensional multiscale approximation of high dimensional problem. 4/16 (Euler, NSF) 7/16 (Grad, Scale Induced Closure)











Beyond Kinetic Theory

Example from Kinetic Theory shows more general abilities of Scale Induced Closure:

$$\mathbf{N}\gg \mathbf{1}$$
 $y'(t)=Ay-rac{1}{arepsilon}By, \qquad y\in \mathbb{R}^N, \qquad B \mbox{ sym. pos. semidef.}$

- Parametrize (low dimensional) ker *B* by ρ , *M*.
- ► Choose accuracy of order $C y = M\rho + \varepsilon G_1^{A,B} \mu_1^{A,B} + \dots + \varepsilon^C G_C^{A,B} \mu_C^{A,B}$
- ▶ Order of Magnitude determines higher moments $\mu_i^{A,B}$, $G_i^{A,B}$ out of A and B, i = 1, ..., C.
- Solve low dimensional system for ρ , $\mu_1^{A,B}$,..., $\mu_C^{A,B}$

General approximation theory without spectral gap but with cascade of scales induced by $1, \varepsilon, \ldots \varepsilon^C$.

Summary

Kinetic Equation: high dimensional, many details

Classical Closures:

Chapman-Enskog: $f = M\rho + \varepsilon f_1 + \varepsilon^2 f_2 + \mathcal{O}(\varepsilon^3)$; equilibrium variables used. \bigoplus accurate, \bigcirc higher orders unstable.

Grad: $f = M\rho + G\mu$; arbitrary direction in phase space. \bigcirc unclear accuracy, \bigoplus stable.

- ♦ Scale Induced Closure: $f = M\rho + \varepsilon G\mu + \mathcal{O}(\varepsilon^2)$, kinetic equation $\longrightarrow G = -K^{\dagger} \mathbf{c} M D^{\dagger}$ \bigoplus accurate, \bigoplus stable.
- Provides equations in transition regime of kinetic theory.
- Can be used for low dimensional approximations of general stiff problems.

Hybrid Approach: Ideas



Problems:

- \blacktriangleright $f(\mathbf{x}, t, \mathbf{c})$ expensive ($\mathbf{c} \in \mathbb{R}^3$)
- Too many details in most situations
- Non-Galilei invariant formulation (moving mesh)

Ideas:

- Use weak formulation, transform to Galilei-invariant form.
- > Approximate $f_{x,t}(c)$ appropriately (moments, point values, Gaussians,...)
- **Couple to conservation laws to guarantee conservation of** ρ , v, θ .

Galilei Invariant, Scaled Formulation

Hybrid Approach

Transfer Equation (Boltzmann equation in weak form): $(\rho\langle\psi\rangle)_t + (\rho\langle c_k\psi\rangle)_{x_k} = m\int f\partial_t\psi dc + m\int fc_k\partial_{x_k}\psi dc + m\int\psi S(f,f)dc$

Moving Mesh:

Rescale
$$c_i$$
 to $\xi_i = \frac{c_i - v_i(\mathbf{x}, t)}{\sqrt{\theta(\mathbf{x}, t)}}$, writing $f(t, x, c) = \hat{f}(t, x, \xi)$.



Galilei invariant! Domain centered around zero. No reduction in resolution.

Note: Cannot get full *f* from \hat{f} (unknown v, θ).

Linking constraints:
$$\int \xi \hat{f} d\xi = 0$$
, $\int \hat{f} d\xi = \frac{\rho}{\sqrt{\theta^d}}$, $\frac{1}{d} \int \xi^2 \hat{f} d\xi = \frac{\rho}{\sqrt{\theta^d}}$

Decomposition of \hat{f}



$$\hat{\mathbf{f}}(t, x, \xi) = \sum_{\beta=1}^{N} \kappa_{\beta}(x, t) \hat{\phi}_{\beta}(\xi)$$

 $\hat{\phi}_{\alpha}(\xi)$ Basisfunctions $\kappa_{\beta}(t,x)$ coefficients.

$$\begin{split} \langle f,g\rangle &:= \int fgd\xi \text{ and } M^{\alpha\beta} = \langle \hat{\phi}_{\alpha}, \hat{\phi}_{\beta} \rangle. \\ &\implies \kappa_{\beta}(t,x) = \sum_{\alpha=1}^{N} (M^{-1})_{\alpha\beta} \int \widehat{\mathbf{f}} \, \hat{\phi}_{\alpha} d\xi \end{split}$$

 $\hat{\phi}$ Gaussian



 $\hat{\phi}$ Piecewise Constants



Hybrid Approach

Transfer Equation for $\kappa_{\alpha}(t, x)$

Rewrite transfer equation, testing with $\hat{\psi}(t, x, \xi) = \frac{1}{\rho(t, x)} \hat{\phi}(\xi)$:

$$(\rho \langle \psi \rangle)_t + (\rho \langle c_k \psi \rangle)_{x_k} = m \int f \partial_t \psi dc + m \int f c_k \partial_{x_k} \psi dc + m \int \psi S(f, f) dc$$

 $\downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow$ 'material equations'

$$\begin{split} M^{\alpha\beta}\partial_{t}\kappa_{\beta} &+ \left[M^{\alpha\beta}v_{k} + M_{k}^{\alpha\beta}\sqrt{\theta}\right]\partial_{x_{k}}\kappa_{\beta} = \\ &+ \left[\left(G_{s,s}^{\alpha\beta}\partial_{t} + \left(G_{s,s}^{\alpha\beta}v_{k} + G_{ks,s}^{\alpha\beta}\sqrt{\theta}\right)\partial_{x_{k}}\right)\ln\left(\theta^{1/2}\right) \\ &+ \frac{1}{\sqrt{\theta}}\left(G_{,j}^{\alpha\beta}\partial_{t} + \left(G_{,j}^{\alpha\beta}v_{k} + \sqrt{\theta}G_{k,j}^{\alpha\beta}\right)\partial_{x_{k}}\right)v_{j} - \frac{1}{\tau}M^{\alpha\beta}\right]\kappa_{\beta}(x,t) \end{array}\right\} \text{relax.} \\ &+ \frac{1}{\tau}\frac{\rho}{(2\pi\theta)^{d/2}}\int\hat{\phi}_{\alpha}(\xi)e^{-\xi_{k}^{2}}d\xi \quad \Big\} \text{source}$$

$$\begin{split} M_{k}^{\alpha\beta} &= \int \xi_{k} \hat{\phi}_{\alpha} \hat{\phi}_{\beta} d\xi, \quad G_{,j}^{\alpha\beta} = \int \hat{\phi}_{\alpha} \, \partial_{\xi_{j}} \, \hat{\phi}_{\beta} d\xi, \quad G_{k,j}^{\alpha\beta} = \int \xi_{k} \hat{\phi}_{\alpha} \, \partial_{\xi_{j}} \, \hat{\phi}_{\beta} d\xi, \\ G_{kj,j}^{\alpha\beta} &= \int \xi_{k} \xi_{j} \hat{\phi}_{\alpha} \, \partial_{\xi_{j}} \, \hat{\phi}_{\beta} d\xi \quad \text{ all pure numbers (indep. of t,x,\xi)} \end{split}$$

Coupling through Heat Flux

Main idea:

Solve closure problem for q in conservation laws by coupling to material equations:

$$q_{k} = m \int (c_{k} - v_{k})(c_{l} - v_{l})^{2} f dc = \sqrt{\theta}^{d+3} \int \xi^{2} \xi_{k} \hat{f} d\xi$$
$$\cong m \sqrt{\theta}^{d+3} \sum_{\beta=1}^{N} \kappa_{\beta}(t, x) \int \xi^{2} \xi_{k} \hat{\phi}_{\beta} d\xi := \sqrt{\theta}^{d+3} \sum_{\beta=1}^{N} \kappa_{\beta} V_{3;k}^{\beta}$$

Define further pure numbers:

Features:

- Enable macro-balance through conservation laws.
- Constraints couple κ_β to macro-level.

$$\begin{split} V_0^{\alpha} &:= \int \hat{\phi}_{\alpha}(\xi) d\xi \\ V_{1;i}^{\alpha} &:= \int \xi_i \hat{\phi}_{\alpha}(\xi) d\xi \\ V_2^{\alpha} &:= \int \xi_k \xi_k \hat{\phi}_{\alpha}(\xi) d\xi \\ V_{\exp}^{\alpha} &:= \int \hat{\phi}_{\alpha}(\xi) e^{-\xi_k^2} d\xi \end{split}$$

Boltzmann U Conservation Laws

Hybrid Approach

Coupled equations in 1+1 dimensions

$$\begin{aligned} &\partial_{t}\rho + \partial_{x}(\rho v) = 0 \\ &\partial_{t}\left(\rho v\right) + \partial_{x}\left(\rho v^{2} + \rho\theta\right) = 0 \\ &\partial_{t}\left(\frac{1}{2}\rho\theta + \frac{1}{2}\rho v^{2}\right) + \partial_{x}\left[\left(\frac{1}{2}\rho\theta + \frac{1}{2}\rho v^{2}\right)v + \rho\theta v + q\right] = 0 \end{aligned} \right\} \quad \text{cons. laws} \\ &\mathbf{q} = \mathbf{m}\theta^{2}\kappa_{\beta}(\mathbf{x}, \mathbf{t})\mathbf{V}_{\mathbf{3};\mathbf{k}}^{\beta} \right\} \quad \text{coupling} \end{aligned}$$

Remarks:

- Use sum convention.
- Matrices M, G, vectors V, are known pure numbers.
- Hyperbolicity?, accuracy?
- Constraints?

Conclusions

Provides equations in transition regime of kinetic theory.

Can be used for low dimensional approximations of general stiff problems.

Kinetic Equation: High detail resolution in all (kinetic) regimes.

- ▶ Galilei-invariant, scaled weak formulation.
- General Decomposition $\hat{f} = \sum_{\beta=1}^{N} \kappa_{\beta}(x, t) \hat{\phi}_{\beta}(\xi)$
- **Coupling** of Boltzmann and Conservation Laws through heat flux q.
- ► Hyperbolicity? Accuracy?

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Engraziel fetg per Vossa attenziun !